Magnetic properties of Fe embedded in V and Cr: Thin films and dilute alloys

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We have calculated the magnetic moment of Fe as a function of the number of nearest V and Cr atoms. We find that the Fe magnetic moment disappears in a neighborhood of exclusively V atoms, but remains larger than $1.85\mu_B$ in a Cr neighborhood. This behavior, which is in excellent agreement with experiment, is a result of the pseudogap formed in the bcc state density. [S0163-1829(97)01501-4]

In the early 1960s Matthias *et al.*[1] and Clogston *et al.*[2] found that Fe impurities are magnetic in Mo, but nonmagnetic in Nb. These experimental findings were confirmed in the late 1980s by Riegel *et al.*,[3] who found that Fe impurities are generally magnetic in group-VIb metals, but nonmagnetic in group-Vb metals. *Ab initio* calculations have reproduced these findings for Fe impurities in Mo and Nb,[4] but we are not aware of any satisfactory explanation of these trends. In the present paper we investigate the magnetic properties of Fe atoms embedded in V and Cr. These systems have attracted considerable attention, but so far only calculations for dilute Fe-based alloys[5–7] or Fe alloys with intermediate concentrations[8,9] have been carried out, while we are interested in the limit of small Fe concentrations.

In an earlier publication, the decrease of the Fe magnetic moment at an Fe surface covered by V or Cr overlayers was explained in terms of the hybridization between the Fe host and the V and Cr *d* bands.[10] Here, we extend this work by calculating the magnetic moment of Fe as a function of the number of V or Cr atoms in its nearest neighborhood. To understand the magnetic behavior of Fe surrounded by either V or Cr, we performed two different sets of calculations. First, we studied a sandwich geometry, where we embedded one or two [100] layers of either pure Fe or an Fe_xV_{1-x} alloy between two semi-infinite body-centered-cubic crystals of V. The Fe-Cr system was treated in a similar manner. By changing the number of Fe monolayers (ML) or/and alloy concentration we modify the number of V or Cr nearest neighbors in the first shell of the Fe atom. For example, in the case of a single Fe ML embedded in a V host all of the eight nearest neighbors of Fe are host (=V) atoms, while for two ML of Fe this number is reduced to 4. Second, we studied bulk Fe_xV_{1-x} and Fe_xCr_{1-x} alloys. In the dilute limit of small x the probability of finding an Fe-Fe pair can be neglected, and thus the number of host V or Cr neighbors in the first Fe shell is again 8.

We have performed self-consistent electronic structure calculations by means of the scalar relativistic spin-polarized Green's-function technique[11] based on the linear muffin-tin orbital (LMTO) method[12,13] within the tight-binding,[14–16] frozen core, and atomic-sphere approximations together with the local spin density approximation as parametrized by Vosko, Wilk, and Nusair.[17] The alloy was treated within the coherent potential approximation (CPA).[18] Our calculations do not take lattice relaxations into account and we assumed atomic spheres of equal radii. For the V-rich and Cr-rich calculations we assumed lattice constants of 3.03 Å and 2.88 Å, respectively, corresponding to the experimental bcc lattice constants of the hosts.

We find, in accordance with earlier calculations and experiments, that the Fe magnetic moment vanishes if all its eight nearest neighbors are V atoms, whereas Fe retains a magnetic moment in a Cr surrounding. In Fig. 1 we show the Fe magnetic moment as a function of the number of its foreign nearest neighbors. The Fe magnetic moment is seen to vanish in the case of one monolayer (ML) of pure Fe or 1 ML of an $Fe_{50}V_{50}$ alloy embedded into bulk V, as well as for a dilute bulk Fe_1V_{99} alloy, i.e., when the number of host V atoms in the first Fe shell is 8. In contrast, when all nearest
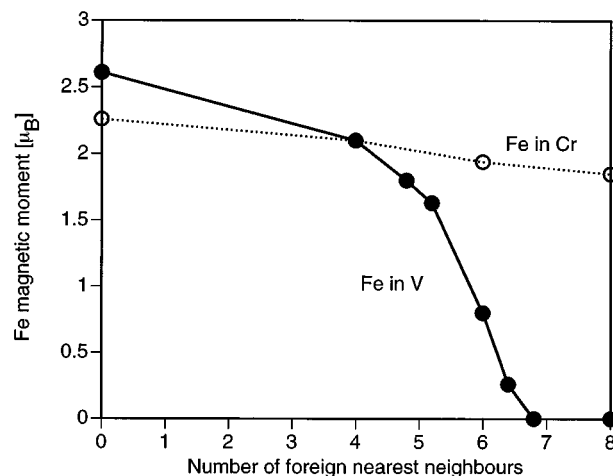

FIG. 1. The Fe magnetic moment as a function of the number of its foreign nearest neighbors given by 4 (2 ML), 4.8 (2 ML, $c=0.8$), 5.2 (2 ML, $c=0.7$), 6.0 (2 ML, $c=0.6$), 6.4 (2 ML, $c=0.5$), 6.8 (2 ML, $c=0.4$), 8.0 ($c=0.01$), and 8.0 (1 ML) where c is the Fe concentration. The solid (dotted) line corresponds to Fe embedded in V (Cr). The small difference in moment between Fe-V and Fe-Cr for no foreign nearest neighbors reflects the difference in the host lattice parameter.
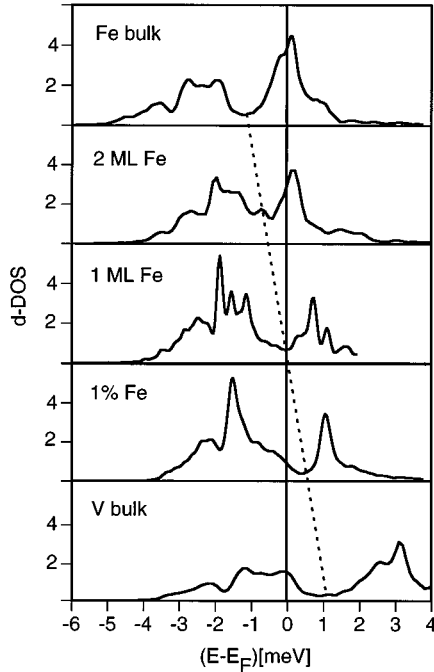
FIG. 2. Paramagnetic Fe d-projected density of states (DOS) for bulk Fe (top), 2 ML of Fe embedded in bulk V, 1 ML of Fe embedded in bulk V, 1% Fe dissolved in bulk V, and bulk V (bottom).

FIG. 3. Paramagnetic Fe d-projected density of states (DOS) for bulk Fe (top), 1 ML of Fe embedded in bulk Cr, 1% Fe dissolved in bulk Cr, and bulk Cr (bottom).

neighbors are Cr atoms Fe retains a finite magnetic moment of $1.85\mu_B$. It is also seen in the figure that the Fe magnetic moment increases linearly with decreasing number of Cr nearest neighbors, whereas in V the Fe magnetic moment shows almost a steplike behavior when the number of foreign nearest neighbors decreases.

In order to explain this change in behavior of the Fe magnetic moment, we present in Figs. 2 and 3 the Fe d-projected paramagnetic densities of state (DOS) for pure Fe (top panel), pure V and Cr (bottom panel), and for Fe atoms embedded into V or Cr (middle panels) with different numbers of foreign nearest neighbors. The most prominent feature of these densities of state is the pseudogap which in bcc metals separate the bonding and antibonding states. In pure Fe the pseudogap, indicated by the dashed line in Figs. 2 and 3, is below the Fermi level which falls at a peak in the antibonding part of the density of states. Hence, the Stoner criterion is satisfied and Fe is ferromagnetic. In pure Cr the Fermi level falls in the middle of the pseudogap and the Stoner criterion is not satisfied. Instead, Cr is antiferromagnetic. Finally, in pure V the pseudogap is above the Fermi level and this metal is neither ferromagnetic nor antiferromagnetic.

We first discuss the densities of state for Fe surrounded by V shown in Fig. 2. Here, we observe that for 1 ML of Fe and the dilute alloy the position of the pseudogap has changed such that the density of states at the Fermi level falls well below the value necessary to satisfy the Stoner criterion. Hence, the ferromagnetic moment disappears (we have so far not investigated the possibility of an antiferromagnetic solution). The difference in the DOS between 1 ML of Fe and the dilute (1% Fe) bulk alloy is due to the different numbers of foreign next-nearest-neighbor atoms, i.e., those atoms which belong to the second shell. Comparing the DOS for the 2
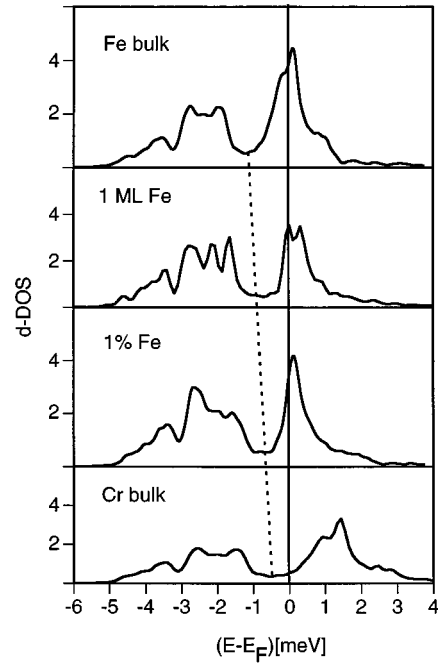
ML, the 1 ML, and the dilute bulk alloy, we find that the entire Fe d band shifts towards higher energies with increasing number of V neighbors. This shift is especially pronounced for the antibonding states and as a result the pseudogap moves up through the Fermi level thereby suppressing ferromagnetism.

In Fig. 3 we show the paramagnetic d-DOS for Fe in a Cr surrounding. In contrast to the V case, the Fe antibonding peak now remains at the Fermi level both for the case of 1 ML of Fe and the 1% alloy. As a result, the Stoner criterion remains satisfied and the magnetic moment at the Fe sites does not vanish.

The change in the position of the pseudogap in both Fe-V and Fe-Cr follows a smoth interpolation between the cases of pure Fe and pure V or Cr. This is not entirely trivial because bulk V and Cr do not correspond to the dilute limit of Fe impurities. The position of the Fe d states may, however, be explained in terms of a two-step model, similar to one used by Friedel.[19] First we observe that the formation of the pseudogap is caused by the geometry of the bcc structure and that the bonding-antibonding splitting of the Fe states remains when Fe is surrounded by V or Cr. Then we note that the potentials of pure V and Cr are less attractive in comparison with bulk Fe, because V and Cr have less nuclear charges than Fe. As a result the perturbed potential on an Fe site will be less attractive compared to pure bulk Fe. The Fe d states will therefore experience a repulsion in a V or Cr surrounding and they will shift to higher energies. This shift in the position of the Fe d band implies that d states occupied in bulk Fe become empty. However, this would lead to an energetically unfavorably large charge transfer and the number of occupied states on the Fe atom therefore remains almost unchanged.[20] The result of the charge conservation and a new, less attractive potential is a shift of mainly the

antibonding peak and the pseudogap towards higher energies. This is essentially what is seen in Figs. 2 and 3.

In summary, we have shown that the magnetic moment of Fe in a V neighborhood approaches zero with increasing number of V neighbors while for Fe in a Cr surrounding the magnetic moment decreases linearly to a value of $1.85\mu_B$. This change in magnetic behavior, which is in agreement with experiments, is a consequence of the formation of a pseudogap in the bcc state density. This picture should also apply to the other Vb and VIb metals.

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